

1,3-Propanediol, diacetate  
628-66-0 | DTXSID30211889

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.12e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.61e-01

Confidence level: 7.65e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,3-Propanediol, diacetate</div> <div>Measured: 6.24e-01</div> <div>Predicted: 4.12e-01</div>	<div>Image not found</div> <div>Propylene glycol diacetate</div> <div>Measured: 6.24e-01</div> <div>Predicted: 3.94e-01</div>	<div>Image not found</div> <div>Dimethyl glutarate</div> <div>Measured: 3.68e-01</div> <div>Predicted: 4.48e-01</div>
<div>Image not found</div> <div>ethyl 2-acetyloxypropanoate</div> <div>Measured: 2.00e-01</div> <div>Predicted: 2.26e-01</div>	<div>Image not found</div> <div>Propanoic acid, 2-(1-oxopropoxy)-, methyl ester</div> <div>Measured: 1.37e-01</div> <div>Predicted: 2.58e-01</div>	